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SIMULATION OF SOLUTE TRANSPORT IN 3D POROUS MEDIA USING RANDOM WALK PARTICLE TRACKING METHOD

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Abstract. Random walk particle tracking (RWPT) method provides a computationally effective way to characterize solute transport process in porous media. In this work, an object-oriented scientific software platform OpenGeoSys (OGS) was adopted for the simulation and visualization of the complex behavior of particles. Finite element method is used for the calculation of the velocity field which is necessary for the determination of the displacement of the particles through space.

The RWPT method has been used in the simulation of the hydraulic process, diffusion and dispersion as it is proved to be well suited for such studies. In this work, efforts were taken to search for the solution to simulate the retardation and decay processes in order to investigate the effects that appear in the contaminant plume evolution. Expressions for the effective coefficients governing the solute transport are derived for retardation model, based on a two-rate sorption-desorption approach.

The RWPT model was first verified by a benchmark test of solute transport in a one-dimensional homogeneous media to analysis the accuracy of the method with comparison to the analytical solution. The analysis was then extended to applications with three-dimensional homogeneous aquifer. This method can be used as a tool to elicit and discern the detailed structure of evolving contaminant plumes.

1 INTRODUCTION

Eulerian and Lagrangian transport models are two basic approaches in numerical simulation of solute transport. The first one has limitations in application of numerical dispersion, thus a higher grid resolution and smaller time steps have to be applied[1]. Whereas the latter avoids solving the transport equation directly, therefore does not need such consideration, the computational times are reduced. But the Lagrangian approach also has disadvantage when applied to dissipative systems. RWPT method was developed basing on the Lagrangian concept. A finite number of particles represent the distribution of the solute mass in porous media and their behavior can be observed[2]. The particles are moved through the porous media according to the velocity field obtained from the solution of the flow equation.

RWPT method has been used for modeling solute transport in aquifers[3], complex, high-resolution transport problems[4, 5], advective-dispersive transport in composite media[6], fractional-order multiscaling anomalous diffusion[7], non-Fickian transport[8].

There are other concepts of particle tracking methods, for instance, continuous time random walk (CTRW)[9, 10, 11], and convolution-based particle tracking (CBPT)[12]. Particle tracking methods have been frequently adopted in the study of flow and solute transport in groundwater modeling. The most common applications are for the delineation of path lines in a flow model. Softwares have the module of particle tracking (MODFLOW), or provide a visualization tool for the path lines and travel times simulation (FEFLOW, ParaView). Most of the researches using particle tracking method only considered the advective-dispersive process, few of them mentioned about retardation and decay. To this purpose, a RWPT model was established on an scientific software platform OpenGeoSys (OGS)[13, 14] as discussed in the following section.

The OGS project is an open source initiative for numerical simulation of thermo-hydro-mechanical-chemical(THMC) processes in porous media. Finite element method was used for the calculation of the velocity field. In the RWPT simulation, a finite number of particles were injected into the calculation domain[15], the mobility of the particles was controlled by using retardation and decay models. The number of particles that leave the domain was counted to produce the breakthrough curves.

2 THEORY

This work made use of the groundwater flow model implemented in OGS[13, 14]. The model deals with saturated subsurface flow. The governing equation for groundwater flow is the fluid mass balance equation. Darcy's law is used for momentum balance.

2.1 Transport Model

The classical advection-dispersion equation of a conservative solute in porous media can be written as[16]

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\boldsymbol{v} C) + \nabla \cdot (\boldsymbol{D} \nabla C) \tag{1}$$

where C is the mass concentration (ML^{-3}), $\boldsymbol{v}$ is the pore velocity vector (ML^{-1}), and $\boldsymbol{D}$ is the hydrodynamic dispersion tensor (L^2T^{-1}), t is time (T^2) and $\nabla$is the differential nabla operator.

2.2 The Random Walk Particle Tracking (RWPT) Method

The RWPT method is issued from stochastic physics. The stochastic differential equation is[17]

$$\mathbf{x}(t_i) = \mathbf{x}(t_{i-1}) + \mathbf{v}(\mathbf{x}(t_{i-1}))\Delta t + Z\sqrt{2\mathbf{D}(\mathbf{x}(t_{i-1}))\Delta t} \tag{2}$$

where $\mathbf{x}$ is the coordinates of the particle location, Δt is the time step, and Z is a random number whose mean is zero and variance is unit.

It has been shown that this equation is equivalent to an expression that is slightly different from the advection-dispersion equation (1). To be equivalent to equation (1), the modified velocity[18] is expressed as

$$\mathbf{v}_i^* = \mathbf{v}_i + \sum_{j=1}^{3} \frac{\partial \mathbf{D}_{ij}}{\partial x_j} \tag{3}$$

with dispersion tensor[16]

$$\mathbf{D}_{ij} = \alpha_T |\boldsymbol{v}| \delta_{ij} + (\alpha_L - \alpha_T) \frac{\mathbf{v}_i \mathbf{v}_j}{|\boldsymbol{v}|} + \mathbf{D}_{ii}^d \tag{4}$$

where δ_{ij} is the Kronecker symbol, α_L is the longitudinal dispersion length, α_T is the transverse dispersivity, D_{ij}^d is the tensor of molecular diffusion coefficient, and $\mathbf{v}_i$ is the component of the mean pore velocity in the ith direction.

The equivalent stochastic differential equation to (1) in three dimensional problems can be written as[4, 19, 20]

$$\begin{aligned}
x_{t+\Delta t} &= x_t + \left(\mathbf{v}_x(x_t, y_t, z_t, t) + \tfrac{\partial D_{xx}}{\partial x} + \tfrac{\partial D_{xy}}{\partial y} + \tfrac{\partial D_{xz}}{\partial z}\right)\Delta t \\
&\quad + \sqrt{2D_{xx}\Delta t}Z_1 + \sqrt{2D_{xy}\Delta t}Z_2 + \sqrt{2D_{xz}\Delta t}Z_3 \\
y_{t+\Delta t} &= y_t + \left(\mathbf{v}_y(x_t, y_t, z_t, t) + \tfrac{\partial D_{yx}}{\partial x} + \tfrac{\partial D_{yy}}{\partial y} + \tfrac{\partial D_{yz}}{\partial z}\right)\Delta t \\
&\quad + \sqrt{2D_{yx}\Delta t}Z_1 + \sqrt{2D_{yy}\Delta t}Z_2 + \sqrt{2D_{yz}\Delta t}Z_3 \\
z_{t+\Delta t} &= z_t + \left(\mathbf{v}_z(x_t, y_t, z_t, t) + \tfrac{\partial D_{zx}}{\partial x} + \tfrac{\partial D_{zy}}{\partial y} + \tfrac{\partial D_{zz}}{\partial z}\right)\Delta t \\
&\quad + \sqrt{2D_{zx}\Delta t}Z_1 + \sqrt{2D_{zy}\Delta t}Z_2 + \sqrt{2D_{zz}\Delta t}Z_3
\end{aligned} \tag{5}$$

where Z_i is the corresponding directional random number.

Together with equation (4), the spatial derivatives of the dispersion coefficients can be expressed as a function of the derivatives of velocity. Note that to obtain the derivatives of velocity, velocity has to be continuous function. For this end, we interpolate velocity at any location in an element from the known velocity at the element nodes.

Since the proposed RWPT method makes use of the FEM for velocity estimation, the derivative of velocity within each element is computed as in Fig. 1 and written as

$$\begin{array}{c} \frac{\partial \mathbf{v}_x}{\partial x} = \frac{\mathbf{v}(x_R)-\mathbf{v}(x_L)}{l_x}; \quad \frac{\partial \mathbf{v}_y}{\partial y} = \frac{\mathbf{v}(y_U)-\mathbf{v}(y_D)}{l_y}; \quad \frac{\partial \mathbf{v}_z}{\partial z} = \frac{\mathbf{v}(z_N)-\mathbf{v}(z_S)}{l_z} \\ \frac{\partial \mathbf{v}_x}{\partial y} = \frac{\partial \mathbf{v}_x}{\partial z} = \frac{\partial \mathbf{v}_y}{\partial z} = \frac{\partial \mathbf{v}_y}{\partial x} = \frac{\partial \mathbf{v}_z}{\partial x} = \frac{\partial \mathbf{v}_z}{\partial y} \simeq 0 \end{array} \tag{6}$$

where x_L and x_R are the intersectional points of the element edges with an extension of a line parallel to the global x axis at which velocities are $\mathbf{v}(x_L)$ and $\mathbf{v}(x_R)$, y_D and y_U are the intersectional points of the element edge from down to up with extension of the line parallel to the global y axis at which velocities are $\mathbf{v}(y_D)$ and $\mathbf{v}(y_U)$, z_S and z_N are the intersectional points of the element edge from south to north with extension of the line parallel to the global z axis at which velocities are $\mathbf{v}(z_S)$ and $\mathbf{v}(z_N)$, and l_x, l_y, and l_z are the length of each intersectional line respectively.

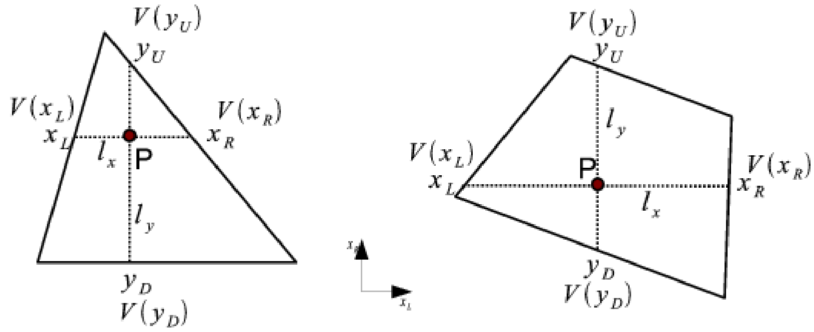


Figure 1: Spatial derivatives of velocity for a particle in triangular and quadrilateral elements

Thus, the derivatives of the dispersion coefficients are as follows[21]

$$\begin{aligned}
\frac{\partial D_{xx}}{\partial x} &= \mathbf{v}_x \frac{\partial \mathbf{v}_x}{\partial x}\left[\alpha_L\left(\frac{2}{\mathbf{v}} - \frac{\mathbf{v}_x^2}{\mathbf{v}^3}\right) - \alpha_T \frac{\mathbf{v}_y^2+\mathbf{v}_z^2}{\mathbf{v}^3}\right] \\
\frac{\partial D_{xy}}{\partial y} &= (\alpha_L - \alpha_T)\left[\frac{\partial \mathbf{v}_y}{\partial y}\frac{\mathbf{v}_x}{\mathbf{v}} - \frac{\mathbf{v}_x \mathbf{v}_y^2}{\mathbf{v}^3}\frac{\partial \mathbf{v}_y}{\partial y}\right] \\
\frac{\partial D_{xz}}{\partial z} &= (\alpha_L - \alpha_T)\left[\frac{\partial \mathbf{v}_z}{\partial z}\frac{\mathbf{v}_x}{\mathbf{v}} - \frac{\mathbf{v}_x \mathbf{v}_z^2}{\mathbf{v}^3}\frac{\partial \mathbf{v}_z}{\partial z}\right] \\
\frac{\partial D_{yy}}{\partial y} &= \mathbf{v}_y \frac{\partial \mathbf{v}_y}{\partial y}\left[\alpha_L\left(\frac{2}{\mathbf{v}} - \frac{\mathbf{v}_y^2}{\mathbf{v}^3}\right) - \alpha_T \frac{\mathbf{v}_x^2+\mathbf{v}_z^2}{\mathbf{v}^3}\right] \\
\frac{\partial D_{yx}}{\partial x} &= (\alpha_L - \alpha_T)\left[\frac{\partial \mathbf{v}_x}{\partial x}\frac{\mathbf{v}_y}{\mathbf{v}} - \frac{\mathbf{v}_y \mathbf{v}_x^2}{\mathbf{v}^3}\frac{\partial \mathbf{v}_x}{\partial x}\right] \\
\frac{\partial D_{yz}}{\partial z} &= (\alpha_L - \alpha_T)\left[\frac{\partial \mathbf{v}_z}{\partial z}\frac{\mathbf{v}_y}{\mathbf{v}} - \frac{\mathbf{v}_y \mathbf{v}_z^2}{\mathbf{v}^3}\frac{\partial \mathbf{v}_z}{\partial z}\right] \\
\frac{\partial D_{zz}}{\partial z} &= \mathbf{v}_z \frac{\partial \mathbf{v}_z}{\partial z}\left[\alpha_L\left(\frac{2}{\mathbf{v}} - \frac{\mathbf{v}_z^2}{\mathbf{v}^3}\right) - \alpha_T \frac{\mathbf{v}_x^2+\mathbf{v}_y^2}{\mathbf{v}^3}\right] \\
\frac{\partial D_{zx}}{\partial x} &= (\alpha_L - \alpha_T)\left[\frac{\partial \mathbf{v}_x}{\partial x}\frac{\mathbf{v}_z}{\mathbf{v}} - \frac{\mathbf{v}_z \mathbf{v}_x^2}{\mathbf{v}^3}\frac{\partial \mathbf{v}_x}{\partial x}\right] \\
\frac{\partial D_{zy}}{\partial y} &= (\alpha_L - \alpha_T)\left[\frac{\partial \mathbf{v}_y}{\partial y}\frac{\mathbf{v}_z}{\mathbf{v}} - \frac{\mathbf{v}_z \mathbf{v}_y^2}{\mathbf{v}^3}\frac{\partial \mathbf{v}_y}{\partial y}\right]
\end{aligned} \tag{7}$$

Because velocity is not derivable at the interface of two adjacent element in a nonuniform flow, computing dispersion coefficient derivatives by using a finite element approach would yield erroneous values[21]. To prevent the errors, a particle is coded to have information of an element index and the velocity estimation is continuous even at the elemental boundaries in this method. Thus, the derivatives of dispersion coefficients will be computed accordingly. This is an improved approach from the work by[21].

3 TRANSPORT IN ONE-DIMENSIONAL SOIL COLUMN

A one-dimensional homogenous aquifer is chosen to simulate a soil column experiment conducted by Harter et al.[22]. In the experiment, a constant flow rate was established, 2.5 pore volumes NaCl - tap water solution and 2.5 pore volumes *Cryptosporidium parvum* solution (1×10^5 oocysts per mL) were injected respectively, the outflow was continuously collected. Fig. 2 shows the schematic description of the experiment.

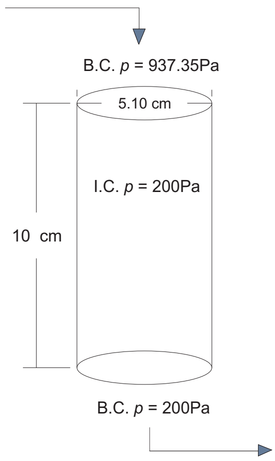


Figure 2: Soil column experiment

NaCl - tap water solution is used as tracer, which experiences only advection and dispersion. The *Cryptosporidium parvum* can be classified as biological colloid. Colloids moving in porous media experience advection, dispersion, sorption-desorption, and filtration.

3.1 Analytical Solution

For one-dimensional transport including sorption-desorption and filtration through a homogeneous medium the following differential equation is applied

$$\frac{\partial C}{\partial t} + \frac{\rho_b}{n}\frac{\partial C_S}{\partial t} = v\alpha_L \frac{\partial^2 C}{\partial x^2} - v(\frac{\partial C}{\partial x} + \lambda C) \tag{8}$$

where C is dissolved concentration ($\mathrm{kg \cdot m^{-3}}$), C_S is sorbed concentration($\mathrm{kg \cdot kg^{-1}}$), t is time (s), ρ_b is bulk density ($\mathrm{kg \cdot m^{-3}}$), n is porosity (-), v is velocity ($\mathrm{m \cdot s^{-1}}$), α_L is longitudinal dispertivity (m), x is distance (m), λ is filtration coefficient (m^{-1}).

The instantaneous, linear sorption model assumes that

$$C_S = K_d C \tag{9}$$

where K_d is the partitioning coefficient ($m^3 \cdot kg^{-1}$). The retardation coefficient R is

$$R = 1 + \frac{\rho_b}{\theta} K_d \tag{10}$$

The dispersion coefficient in x-direction D_{xx} ($m^2 \cdot s^{-1}$) is

$$D_{xx} = v\alpha_L \tag{11}$$

The analytical solution for a pulse input (inject time from 0 to τ) is

$$\begin{aligned} C = \ & \tfrac{1}{2}C_0\Bigg[\exp\left(\frac{vx(1-\gamma)}{2D_{xx}}\right)\operatorname{erfc}\left(\frac{x - v\gamma t/R}{2\sqrt{D_{xx}t/R}}\right) \\ & + \exp\left(\frac{vx(1+\gamma)}{2D_{xx}}\right)\operatorname{erfc}\left(\frac{x + v\gamma t/R}{2\sqrt{D_{xx}t/R}}\right)\Bigg] \end{aligned} \tag{12}$$

for $t \in (0, \tau)$,

$$\begin{aligned} C = \ & \tfrac{1}{2}C_0\Bigg[\exp\left(\frac{vx(1-\gamma)}{2D_{xx}}\right)\operatorname{erfc}\left(\frac{x - v\gamma t/R}{2\sqrt{D_{xx}t/R}}\right) \\ & + \exp\left(\frac{vx(1+\gamma)}{2D_{xx}}\right)\operatorname{erfc}\left(\frac{x + v\gamma t/R}{2\sqrt{D_{xx}t/R}}\right) \\ & - \exp\left(\frac{vx(1-\gamma)}{2D_{xx}}\right)\operatorname{erfc}\left(\frac{x - v\gamma (t-\tau)/R}{2\sqrt{D_{xx}(t-\tau)/R}}\right) \\ & - \exp\left(\frac{vx(1+\gamma)}{2D_{xx}}\right)\operatorname{erfc}\left(\frac{x + v\gamma (t-\tau)/R}{2\sqrt{D_{xx}(t-\tau)/R}}\right)\Bigg] \end{aligned} \tag{13}$$

for $t \in (\tau, \infty)$, where

$$\gamma = \sqrt{1 + 4v\lambda R D_{xx}/v^2} \tag{14}$$

3.2 Numerical Solution

The calculation area is simplified to a line with the length of 0.1m. For the numerical model 100 elements and 101 nodes are included. Head gradient is set by giving two constant pressures at both left and right boundaries to establish a uniform velocity field with the value of 7.1 md^{-1}.

The number of pore volume (x-axis) is calculated by

$$P_V = \frac{vt}{L} \tag{15}$$

where v is the seepage velocity, L is the length of the soil column. The time step size is set by assigning P_V to 0.01. In the simulation, 100 particles per time steps are loaded near the left boundary for 250 time steps.

The filtration process is described by using the filtration coefficient. The sorption-desorption process is described by the two-rate model from Johnson et al.[23]. In the two-rate model, desorption is governed by two different rate coefficients

$$N/N_0 = Ae^{-k_1 t} + (1-A)e^{-k_2 t} \tag{16}$$

where N is the number of particles remaining on the medium at time t, N_0 is the initial number of particles on the medium at the time of initial sorption, A is a weighting factor, k_1 and k_2 are the fast and slow sorption rate coefficient, respectively. Relative parameters are listed in Tab. 1.

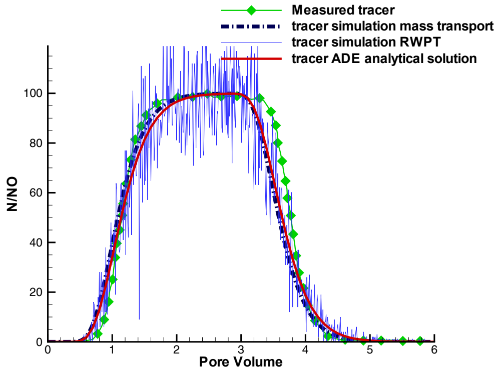
Table 1: Model parameters for the column experiment

Symbol	Parameter	Value	Unit
k	Permeability	1.114476^{-11}	m^2
α_L	Longitudinal dispersion length	0.005	m
n	Porosity(tracer)	0.5	–
n	Porosity(colloid)	0.42	–
A	Weighting factor	0.9	–
k_1	Fast sorption rate coefficient	0.1	–
k_2	Slow sorption rate coefficient	0.001	–
λ	Filtration coefficient	5.2	m^{-1}

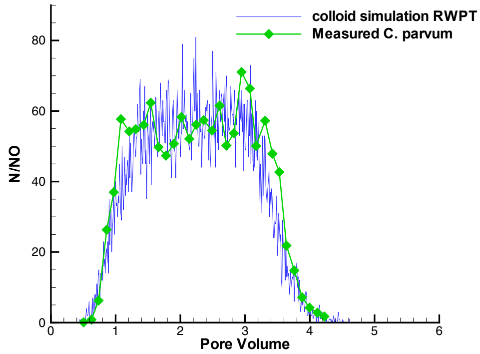
3.3 Results

The tracer experiences only advection and dispersion, which means in Equation (8), $C_S = 0$, $\lambda = 0$. The results of RWPT simulation for the distribution of concentration over time are compared to those of measured value from the experiment by Harter[22], the analytical solution, and the OGS simulation with mass transport method. The comparison results are shown in Fig. 3a. The curves fit very well, which indicates the accuracy of this method.

In the colloid transport simulation, the number of particles leaving the right boundary was counted each time step. The number was then converted to concentration in order to obtain the corresponding breakthrough curve over time. The comparison with the measured value from the experiment by Harter are shown in Fig. 3b. There are five sections in the breakthrough curve, namely the point at which solute is observed, breakthrough, steady state plateau, elution portion, and a persistent tailing. The RWPT method successfully simulated both portions of the curve. The result shows that the method is capable for producing accurate concentrations.



(a) Advection and dispersion

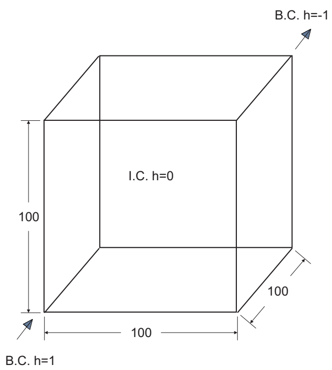


(b) Sorption-desorption and decay

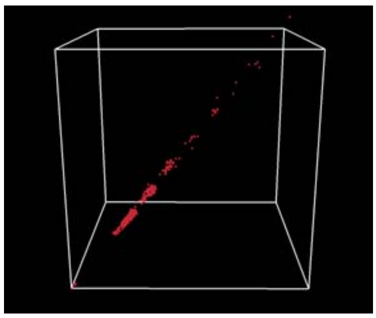
Figure 3: Colloid transport in a soil column

4 TRANSPORT IN THREE-DIMENSIONAL CUBE

A three-dimensional homogeneous cube is chosen to verify advective dispersive transport. The side length of the cube model domain is 100 m. The velocity field is held constant in the diagonal direction from bottom left to top right (Fig. 4a).



(a) Cube schematic



(b) Particle clouds

Figure 4: Particle tracking with advection and dispersion in a cube

4.1 Analytical Solution

The stated problem can be compared with an analytical solution provided by[24].

$$C(x,y,z,t) = \frac{C_0 V}{8(\pi t)^{3/2}\sqrt{D_{xx}D_{yy}D_{zz}}}\exp\left[-\frac{(x-x_0)^2}{4D_{xx}t} - \frac{(y-y_0)^2}{4D_{yy}t} - \frac{(z-z_0)^2}{4D_{zz}t}\right] \quad (17)$$

where C_0 is the initial concentration.

4.2 Numerical Solution

The domain is discretized with tetrahedral elements. The same grid density is used for converting particle distributions to element concentrations. The head gradient is set by assigning two constant boundary conditions on the diagonal joint points.

The initial source load is applied to an area close to the bottom left of the domain to have an initial concentration of $C_0 = 1\ kgm^{-3}$. The material properties for this model setup are given in Tab. 2.

Table 2: Material properties

Symbol	Parameter	Value	Unit
k	Permeability	6.0804^{-10}	m^2
α_L	Longitudinal dispersion length	0.005	m
α_T	Transverse dispersivity	0.005	m
n	Porosity	0.2	–

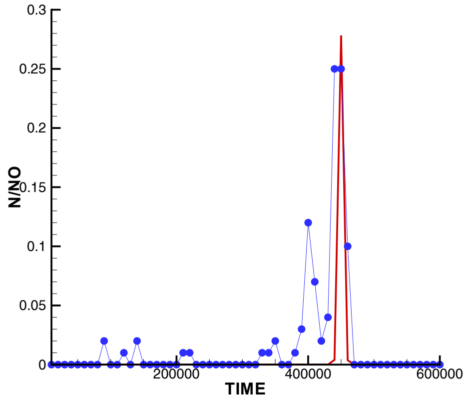
4.3 Results

The advection-dispersion of the particles pulse across the cube is shown in Fig. 4b. The number of particles used for this simulation is 500. Boundary control was applied in the simulation that when a particle reached the surface of the cube, it would be attached. When particles reached the top right point, the number was counted to generate the breakthrough curves.

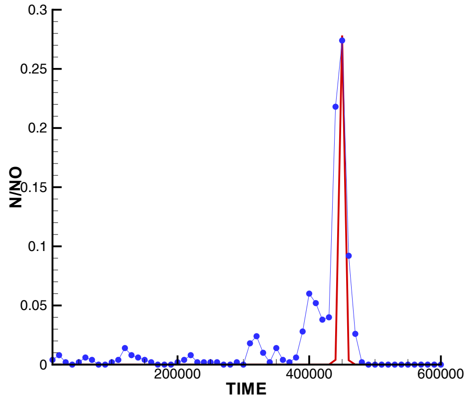
The result of RWPT simulation for the distribution of concentration over time is compared to the analytical solution. The simulations with various numbers of particles are depicted in Fig. 5. We found that 500 particles are sufficient in this case to fit both maximum and breakthrough time, which saves computation time. Computation time is linear relative with the number of particles according to the simulation we applied.

5 CONCLUSIONS

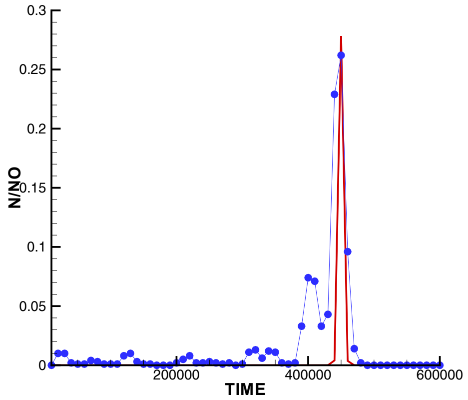
In this work, RWPT model established on the platform OGS was demonstrated. The method was verified by a benchmark test of solute transport in a one-dimensional homogeneous aquifer. We showed that the method can be adopted to simulate the process of retardation and decay as



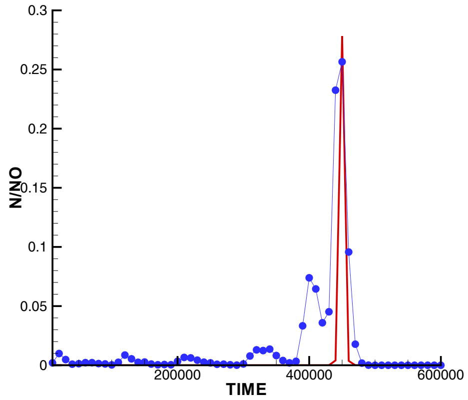
(a) NO=100



(b) NO=500



(c) NO=1000



(d) NO=10000

Figure 5: RWPT simulation in 3D cube compared with analytical solution (solid line)

well as advective-dispersive process. In addition, the method was extended to application in 3D porous media. The RWPT model produced the results in good agreement with the analytical solutions. It is well suited for the simulation of solute transport in saturated porous media. Furthermore, it can be used as a tool to observe the individual behavior of the solute mass with the post-processing.

With this fundamental, adapting the method to the simulation of solute transport in heterogeneous aquifer, coupled flow processes and multiphase flow are currently under development. The method will be applied in real field as well[25].

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